

A Perturbative Expansion for Weakly Bound States*

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Abstract

We describe a perturbation expansion for the energy and wave function of a weakly bound particle in a short-range potential in one space dimension.

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1 Introduction

In this article, we discuss a method for calculating energies and wave functions for weakly bound particles in short range potentials in one dimensional nonrelativistic quantum mechanics. We usually think of the formation of a bound state as a non-perturbative process, however, we will see that for a weakly bound state, with a wave function that extends far outside the region in which the potential is important, we can calculate bound state properties in perturbation theory. In one dimension, the perturbation expansion completely determines the energy and wave function of the state. The expansion is quite simple (closely related to the Born series) and it may well appear somewhere in the literature, but we have been unable to find it.

A particle moving in a generic short range potential has two natural length scales: a , the range of the potential, and κ^{-1} , the size of the state, related to the binding energy, E_0 , of the system by $\kappa = \sqrt{-2mE_0}$.¹ In turn, these scales define a dimensionless parameter, κa . A weakly bound state, one for which $\kappa a \ll 1$, inherently has a small dimensionless parameter which could serve as the basis for a perturbative description of the wave function. In the following, we show that in one dimension we can construct a power series in κa for both the energy and (in a sense) the wave function, assuming that $\kappa a \ll 1$.²

The perturbative expansion that emerges is a series of n coupled integrals with n powers of the potential and $n - 1$ coupling terms at each order of the power series. These terms manifestly respect translation invariance—if the potential is translated in space, the wave function moves correspondingly. For simple potentials, the analytic behavior of the expansion for the bound states can easily be extracted to several orders. We illustrate the procedure for a classic square well potential in order to demonstrate the agreement of the perturbative approach with the known form of the ground state. Less simple potentials can be handled numerically.

Our goal is eventually to extend this perturbative approach to three dimensions and from there to fully relativistic systems. The extension of these one dimensional results to three is not as straightforward as might be hoped. The particle's wave function varies significantly where the potential is large, making the unraveling of the leading κa behavior considerably more difficult. Moreover, the

¹Throughout this article, we use units in which $\hbar = 1$.

²The situation in three dimensions is much more complicated. This condition is replaced by an integral condition on the potential—the small parameter then is the deviation of the actual potential from this condition.

form of the free particle Green's function in three dimensions, unlike its one dimensional analogue, is singular in its first term when expanded in powers of κa . In this note, however, we set aside these difficulties and turn our attention to the particle in one dimension, where the expansion is simple and elegant.

2 The Perturbative Expansion

In the limit that the potential is very short range, we expect that it can be approximated by a δ -function:

$$V(x) \rightarrow v \delta(x) \quad (2.1)$$

where

$$v = \int dx V(x). \quad (2.2)$$

The δ -function potential has a single bound-state, of the form

$$\psi(x) \propto e^{-\kappa|x|} \quad (2.3)$$

where

$$\kappa = -mv \quad (2.4)$$

We seek a systematic expansion in which (2.1)-(2.4) is the first term. Note that because $\kappa \propto V(x)$, we expect that an expansion in powers of κa will be an expansion in powers of V as well. A simple expansion of the Fourier transform of $V(x)$ in powers of the momentum is not suitable because the higher order terms, derivatives of δ -functions, are too singular. Instead, we will exploit the relation between the ground state of the δ -function potential and the free particle Green's function, G_κ :

$$G_\kappa(x) = \frac{e^{-\kappa|x|}}{2\kappa}. \quad (2.5)$$

In integral form, the Schrödinger equation reads

$$\psi(x) = - \int dx' G_\kappa(x - x') 2mV(x')\psi(x') \quad (2.6)$$

where κ is related to the energy of the state, E_0 , by

$$\kappa = \sqrt{-2mE_0}. \quad (2.7)$$

The weakly bound regime occurs when $\kappa a \ll 1$ where a is the range of the potential.

If the argument of the Green's function is small compared to $1/\kappa$, we can legitimately expand the exponential in equation 2.5. In general, in (2.6), this is not true. However, if we multiply (2.6) by $V(x)$, then we get an integral equation for the product, $V(x)\psi(x)$:

$$V(x)\psi(x) = -V(x) \int dx' G_\kappa(x-x') 2mV(x')\psi(x'). \quad (2.8)$$

In (2.8), the short range of the potential guarantees that can do this expansion because the $x-x'$ in the Green's function is sandwiched between $V(x)$ and $V(x')$, so $|x-x'|$ cannot get much larger than a .

By adding and subtracting 1 from the exponential in G_κ , we can rewrite (2.8) as

$$\begin{aligned} V(x)\psi(x) &= -\frac{mV(x)}{\kappa} \int dx' V(x')\psi(x') \\ &\quad -\frac{mV(x)}{\kappa} \int dx' \left[e^{-\kappa|x-x'|} - 1 \right] V(x')\psi(x'). \end{aligned} \quad (2.9)$$

Since the principal contribution to the second integral comes only from the region $x, x' \leq a$, the second term on the right hand side of (2.9) is explicitly suppressed by a factor of κa relative to the first. The expression $\int dx' V(x')\psi(x')$ appears as a factor in all the terms when $V(x)\psi(x)$ is expanded to an arbitrary order so it is to convenient to work from the start instead with the normalized function

$$\chi(x) \equiv \frac{V(x)\psi(x)}{\int dx' V(x')\psi(x')} \quad (2.10)$$

satisfying

$$\int dx \chi(x) = 1. \quad (2.11)$$

In terms of χ , we have

$$\chi(x) = -\frac{mV(x)}{\kappa} - \frac{mV(x)}{\kappa} \int dx' \left[e^{-\kappa|x-x'|} - 1 \right] \chi(x'). \quad (2.12)$$

This expression for $\chi(x)$ serves as the basis for our perturbation series.

2.1 The Energy

From the power series for $\chi(x)$ in equation 2.12, we can obtain an expression for the bound state energy by applying the normalization condition, (2.11). For example, simply neglecting the second term in (2.12) and imposing (2.11) yields

$$1 = \int dx \frac{mV(x)}{\kappa} \quad (2.13)$$

which is equivalent to (2.4). Indeed, for a δ -function potential, the second term in (2.12) vanishes, thus (2.13) is exact, and we reproduce the solution (2.3).

Iterating (2.12) once and neglecting terms of order $m^3 V^3$ yields

$$\chi(x) = -\frac{mV(x)}{\kappa} + 2mV(x) \int dx_1 \left[\frac{e^{-\kappa|x-x_1|} - 1}{2\kappa} \right] \frac{mV(x_1)}{\kappa}. \quad (2.14)$$

The leading contribution to χ is

$$\chi(x) = -\frac{mV(x)}{\kappa} - \frac{m^2 V(x)}{\kappa} \int dx_1 |x - x_1| V(x_1) + \dots \quad (2.15)$$

for which the normalization condition determines the energy to be

$$\kappa = -m \int dx V(x) - m^2 \int dx_1 dx_2 |x_1 - x_2| V(x_1) V(x_2) + \dots \quad (2.16)$$

It is straightforward to continue the expansion to higher order. The expression up to fourth order for κ is given in the appendix, in equation A.24.

Although the terms begin to proliferate as we expand to higher orders, the set of integrals that contribute with an overall coefficient of m^n can be described. The set consists of all *inequivalent* integrals that contain n integrations, n factors of the potential, and $n - 1$ factors of the form $|x_j - x_{j+1}|^{m_j}$ where the sum of the exponents satisfies $\sum_{j=1}^{n-1} m_j = n - 1$. Since the $|x_j - x_{j+1}|^{m_j}$ arises from our expansion of the Green's function, (2.5), it is accompanied by a $(1/m_j!)$. Thus, general n -th order term looks like

$$-m^n s \int \left(\prod_{i=1}^n dx_i V(x_i) \right) \left(\prod_{j=1}^{n-1} \frac{1}{m_j!} |x_i - x_{i+1}|^{m_j} \right). \quad (2.17)$$

There only remains the factor s to explain. In demanding that the integrals be inequivalent, we have slightly undercounted, and the s corrects for this omission. A specific contribution to (2.17) often contains several connected integrals and with each such piece written as

$$\int dx_1 \dots dx_{k \leq n} |x_1 - x_2|^{m_1} |x_2 - x_3|^{m_2} \dots |x_{k-1} - x_k|^{m_{k-1}} V(x_1) \dots V(x_k). \quad (2.18)$$

$s - 1$, then, counts the number of non-trivial ways of rearranging the m_j 's within this connected factor which yield different integrands but the same integral. Similarly, if our term (2.17) contains several connected integrals, the total s is the product of these symmetry factors for each connected component. For example, at fourth order, shown in appendix equation (A.24), we have a term of the form,

$$\left(\int dx V(x) \right) \left(\int dx_1 dx_2 dx_3 |x_1 - x_2|^2 |x_2 - x_3| V(x_1) V(x_2) V(x_3) \right). \quad (2.19)$$

The exponents of the second connected piece could be switched so that the integrand has $|x_1 - x_2||x_2 - x_3|^2$ instead of $|x_1 - x_2|^2|x_2 - x_3|$; but both integrals are equivalent. Thus for (2.19), $s = 2$ (which cancels the $1/2!$ from the Green's function expansion).

2.2 The Wave Function

The expression for $\chi(x)$ to any order contains an explicit factor of $V(x)$. One might think, from (2.10), that we could simply cancel this factor and get the wave function up to a normalization factor. This is not quite right, because the resulting series only converges for small x . However, we can construct the wave function for all x using (2.6), which can be written as

$$\psi(x) = N \int dx' e^{-\kappa|x-x'|} \chi(x') \quad (2.20)$$

where N is a normalization factor.

3 Example: The Square Well Potential

For the square well potential,

$$V(x) = \begin{cases} -V_0 & \text{for } |x| \leq a \\ 0 & \text{for } |x| > a \end{cases} \quad (3.21)$$

our expansion is in powers of the dimensionless quantity,

$$2mV_0a^2. \quad (3.22)$$

If we apply (A.24), we find

$$\begin{aligned} \kappa a = & (2mV_0a^2) - \frac{2}{3}(2mV_0a^2)^2 + \frac{4}{5}(2mV_0a^2)^3 \\ & - \frac{368}{315}(2mV_0a^2)^4 + \mathcal{O}((2mV_0a^2)^5) + \dots \end{aligned} \quad (3.23)$$

which agrees with what we get from a Taylor expansion of the exact value of κ .

Rather than show the rather complicated formulae for the expansion of the wave function, we will display, in figures 1-4, plots of the exact wave function along with the first four approximates, for various values of $2mV_0a^2$. Evidently, for $2mV_0a^2 = 0.3$, shown in figure 1, the expansion for the wave function converges rapidly, while for $2mV_0a^2 = 0.9$, shown in figure 4, the expansion is not working at all.

Acknowledgements

We are very grateful to David Kaplan for many interesting conversations.

A Appendix: Expansion Formulae

This appendix lists the energy and χ expansions to several orders in mV ; the structure of the collection of terms present at a particular order in the κa expansion has been described in section 2.

$$\begin{aligned}
\kappa = & -m \int dx V(x) - m^2 \int dx_1 dx_2 |x_1 - x_2| V(x_1) V(x_2) \\
& - m^3 \left[\int dx_1 dx_2 dx_3 |x_1 - x_2| |x_2 - x_3| V(x_1) V(x_2) V(x_3) \right. \\
& \quad \left. + \frac{1}{2} \left(\int dx V(x) \right) \left(\int dx_1 dx_2 |x_1 - x_2|^2 V(x_1) V(x_2) \right) \right] \\
& - m^4 \left[\int dx_1 dx_2 dx_3 dx_4 |x_1 - x_2| |x_2 - x_3| |x_3 - x_4| V(x_1) V(x_2) V(x_3) V(x_4) \right. \\
& \quad \left. + \left(\int dx V(x) \right) \left(\int dx_1 dx_2 dx_3 |x_1 - x_2|^2 |x_2 - x_3| V(x_1) V(x_2) V(x_3) \right) \right. \\
& \quad \left. + \frac{1}{2} \left(\int dx_1 dx_2 |x_1 - x_2|^2 V(x_1) V(x_2) \right) \left(\int dx_1 dx_2 |x_1 - x_2| V(x_1) V(x_2) \right) \right. \\
& \quad \left. + \frac{1}{6} \left(\int dx V(x) \right)^2 \left(\int dx_1 dx_2 |x_1 - x_2|^3 V(x_1) V(x_2) \right) \right] \\
& + \mathcal{O}(m^5 V^5)
\end{aligned} \tag{A.24}$$

$$\begin{aligned}
& -\kappa\chi(x_1) = m V(x_1) + m^2 \int dx_2 |x_1 - x_2| V(x_1)V(x_2) \\
& + m^3 \left[\int dx_2 dx_3 |x_1 - x_2| |x_2 - x_3| V(x_1)V(x_2)V(x_3) \right. \\
& \quad \left. + \frac{1}{2} \left(\int dx_2 |x_1 - x_2|^2 V(x_1)V(x_2) \right) \left(\int dx V(x) \right) \right] \\
& + m^4 \left[\int dx_2 dx_3 dx_4 |x_1 - x_2| |x_2 - x_3| |x_3 - x_4| V(x_1) V(x_2) V(x_3) V(x_4) \right. \\
& \quad + \frac{1}{2} \left(\int dx_2 dx_3 |x_1 - x_2| |x_2 - x_3|^2 V(x_1)V(x_2)V(x_3) \right) \left(\int dx V(x) \right) \\
& \quad + \frac{1}{2} \left(\int dx_2 dx_3 |x_1 - x_2|^2 |x_2 - x_3| V(x_1)V(x_2)V(x_3) \right) \left(\int dx V(x) \right) \\
& \quad + \frac{1}{2} \left(\int dx_2 |x_1 - x_2|^2 V(x_1)V(x_2) \right) \left(\int dx_2 |x_1 - x_2| V(x_1)V(x_2) \right) \\
& \quad \left. + \frac{1}{6} \left(\int dx_2 |x_1 - x_2|^3 V(x_1)V(x_2) \right) \left(\int dx V(x) \right)^2 \right] \\
& + \mathcal{O}(m^5 V^5)
\end{aligned} \tag{A.25}$$

References

- [1] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, Pergamon Press Ltd., Oxford, 1977.

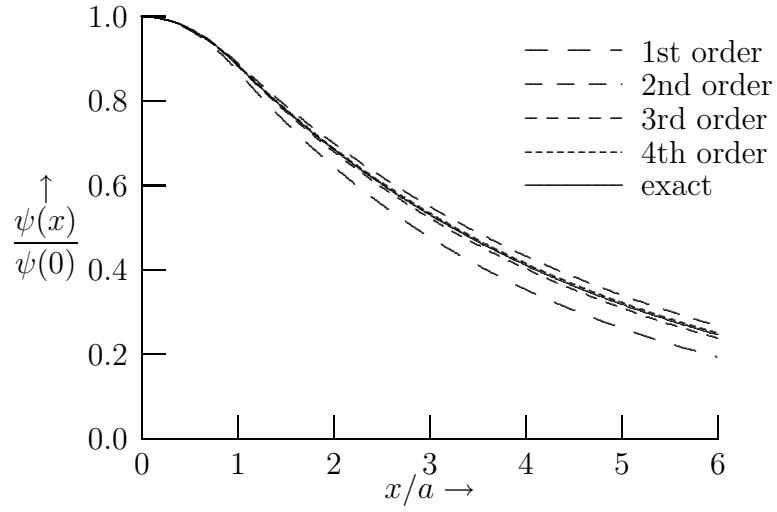


Figure 1: $2mV_0a^2 = 0.3$

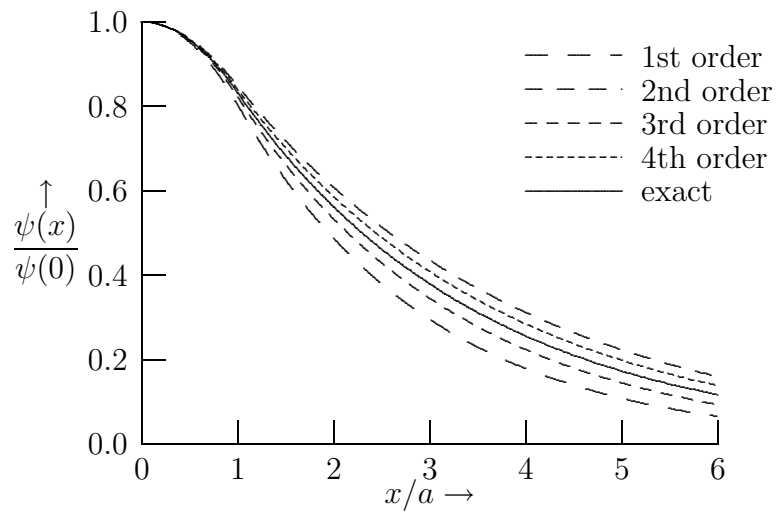


Figure 2: $2mV_0a^2 = 0.5$

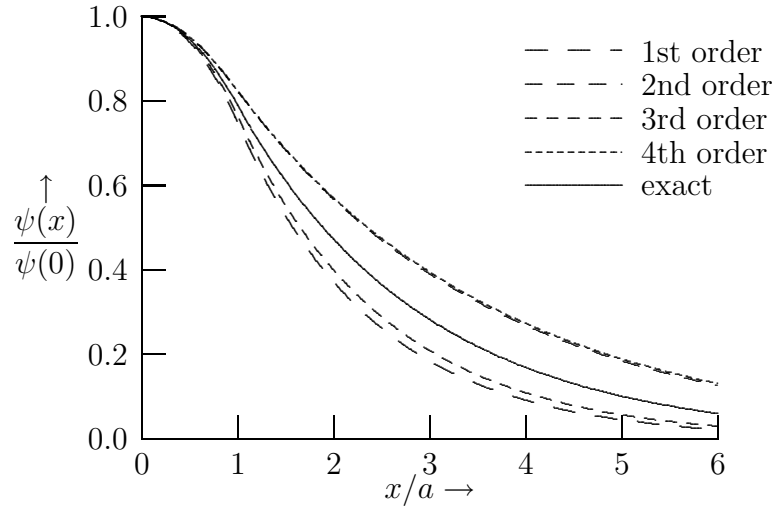


Figure 3: $2mV_0a^2 = 0.7$

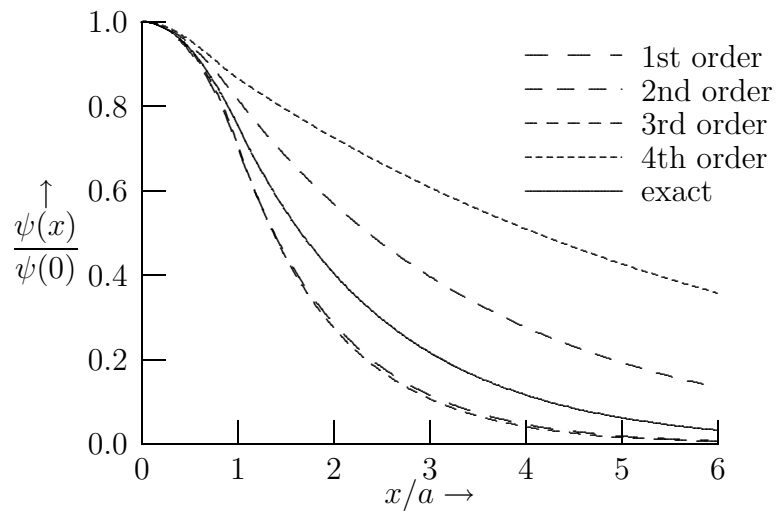


Figure 4: $2mV_0a^2 = 0.9$